

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

Applicant: Harold E. Helson Confirmation No.: 4787  
Application No.: 09/502,133 Art Unit: 2128  
Filed: February 11, 2000 Examiner: H. M. Jones  
Title: ENHANCING STRUCTURE DIAGRAM GENERATION

Commissioner for Patents  
P.O. Box 1450  
Alexandria, VA 22313-1450

**DECLARATION UNDER 37 C.F.R. § 1.132**

Dear Sir:

I, Dr. Harold Helson, declare as follows.

1. I have studied or worked in the areas of chemistry and/or computational chemistry since 1978. A brief description of my education and relevant work experience includes: B.A. (Chemistry), 1983, University of California (Berkeley); Ph.D. (Chemistry), 1993, Purdue University; Postdoctoral work (Dept. of Chemistry) 1993-1994, Yale University. I am currently employed by CambridgeSoft, Inc., and have been since 1994, which is the assignee of the above-captioned patent application (the "133 Application"). My position at CambridgeSoft is Director, Computational Chemistry, a position I have held since 2000. In this capacity, my general responsibilities include representing chemistry in software and providing two-dimensional chemical perception algorithms. I also am the inventor the '133 Application.

2. I have reviewed the '133 Application and the Office Action issued by the Examiner dated September 2, 2009, for the '133 Application.

3. I have been informed that pending claims 1, 9, and 13-35 have been rejected in the latest Office Action under 35 U.S.C. § 103(a) as purportedly being unpatentable over Helson, "Simulation of Carbene Chemistry and Other Problems in Computer-Assisted Organic Synthesis", Purdue University 1993 (herein Helson) in view of Benecke, C., *et al.*, "MOLGEN+, a generator of connectivity isomers and stereoisomers for molecular structure elucidation", *Anal. Chim. Acta*, Vol. 314, pp. 141-147, 1995 (herein Benecke) and the taking of official notice. Specifically, I have been informed that Benecke has been alleged to disclose the laying out of atoms and/or bonds to express symmetry.

4. I have read and understood Benecke.

5. Benecke describes a structure generator software application, MOLGEN+, which produces all of the molecular graphs that correspond to a given chemical formula. As disclosed in Benecke, MOLGEN+ takes as its input a chemical formula, (optionally) prescribed and forbidden substructures, an interval for allowed ring sizes, and maximal bond multiplicities. From this input, MOLGEN+ generates a complete list of all mathematically possible molecular graphs that are compatible with the chemical formula. After generation of the constitutional isomers, MOLGEN+ produces a sketch of the molecules in the form of a tapestry of several molecules shown together or as a single molecule.

6. Benecke states, "MOLGEN+ is capable of generating all possible configurational isomers, again redundancy free (which also implies the consideration of symmetries)." In my opinion, one having skill in the art of computer-based chemical structure diagram generation would understand this statement to mean that symmetries were considered to avoid duplications and missing objects when generating all permutations of a list of elements.

7. In my opinion, one having ordinary skill in the art of computer-based chemical structure diagram generation would not understand Benecke as disclosing or suggesting the laying out of symmetrically equivalent atoms and bonds in a chemical structure diagram to visually express the identified symmetry in a stylized two-dimensional pictorial representation of a chemical structure.

8. The invention being claimed requires identifying an instance of chemical structural symmetry in a chemical structure and laying out symmetrically equivalent atoms and bonds in a chemical structure diagram to visually express the identified symmetry in a stylized two-dimensional pictorial representation of the chemical structure.

9. In my opinion, the claimed invention would not be obvious in light of Helson and Benecke because the combined references do not teach or suggest laying out symmetrically equivalent atoms and bond in a chemical structure diagram to visually express the identified symmetry in a stylized two-dimensional pictorial representation of the chemical structure.

10. I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements are made with the knowledge that willful false statements so made are punishable by fine or imprisonment or both under § 1001 of Title 18 of the United States Code and that such willful statements may jeopardize the validity or enforceability of the present application or any patent issued thereon.

Harold E. Helson  
Dr. Harold E. Helson

3/1/2010  
Date